

Research and Applications of Scientific Visualization

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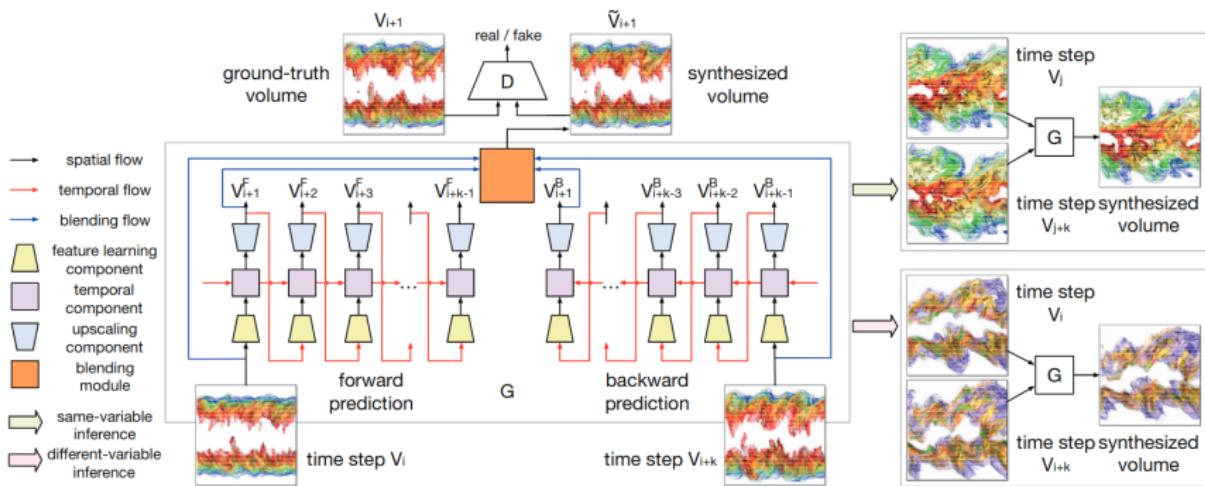
Outline

- ▶ Research Topic: Machine Learning Solving HPC Problems
- ▶ Application: HPC Simulations to Enhance Drug Delivery Designs

TSR-TVD: Temporal Super-Resolution for Time-Varying Data Analysis and Visualization

- ▶ HPC has issues with storing time-steps.
- ▶ Some researchers LERP between time-steps to find intermediate data.
- ▶ TSR-TVD is a machine learning implementation to synthesize timesteps.
- ▶ Researchers are modifying existing ML techniques to solve problems in HPC.
- ▶ <https://ieeexplore.ieee.org/document/8802285>

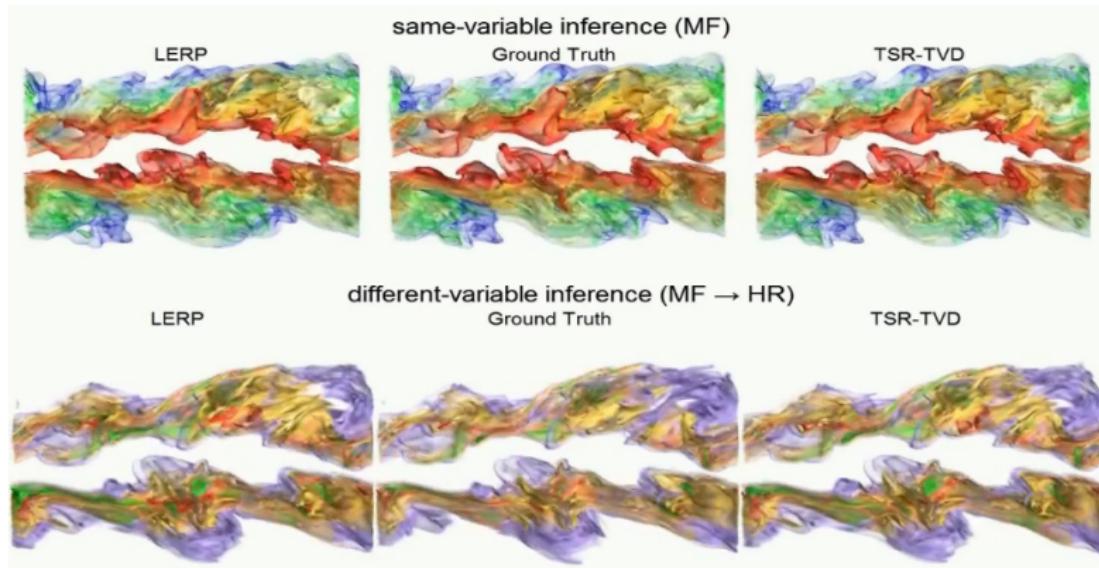
TSR-TVD: Temporal Super-Resolution for Time-Varying Data Analysis and Visualization



TSR-TVD: Temporal Super-Resolution for Time-Varying Data Analysis and Visualization

- ▶ Uses bidirectional RNN to create forward and backward predictions
- ▶ Conv3D GAN adversarially trains network using 3D data.
- ▶ TSR-TVD uses structure similar to TecoGAN.
- ▶ Still needs work, but exciting avenue of research.

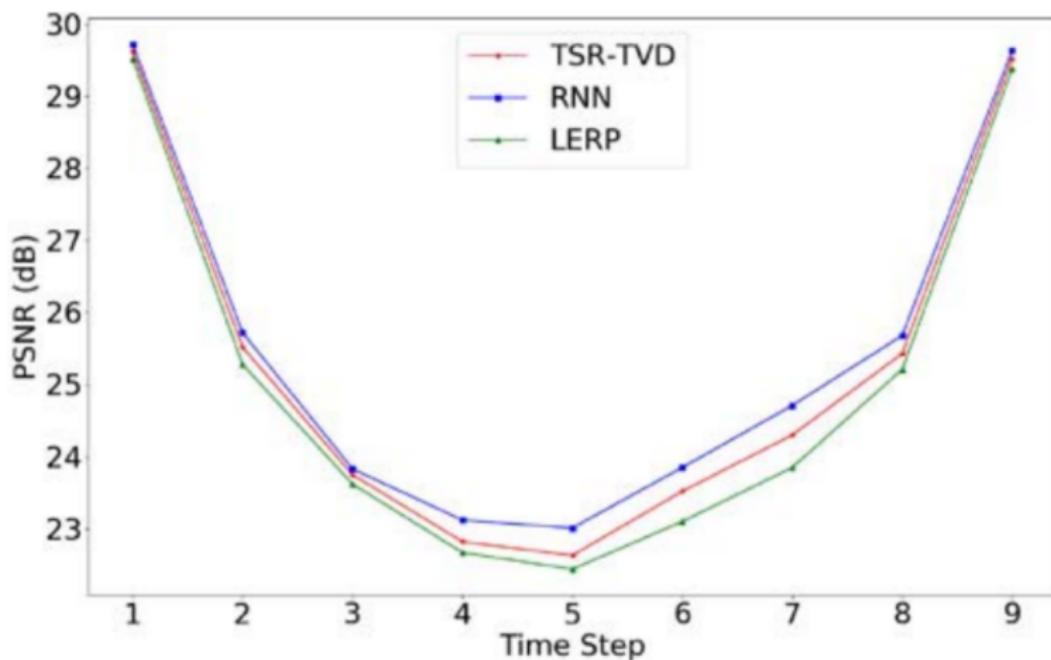
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Short Video

<https://vimeo.com/359998660>

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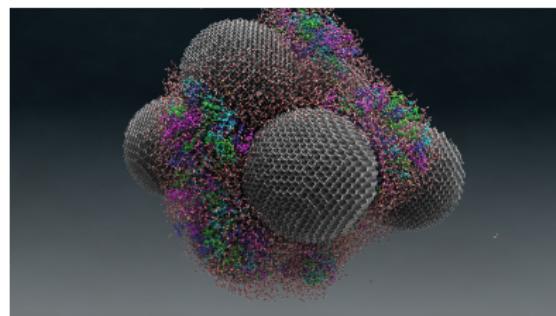


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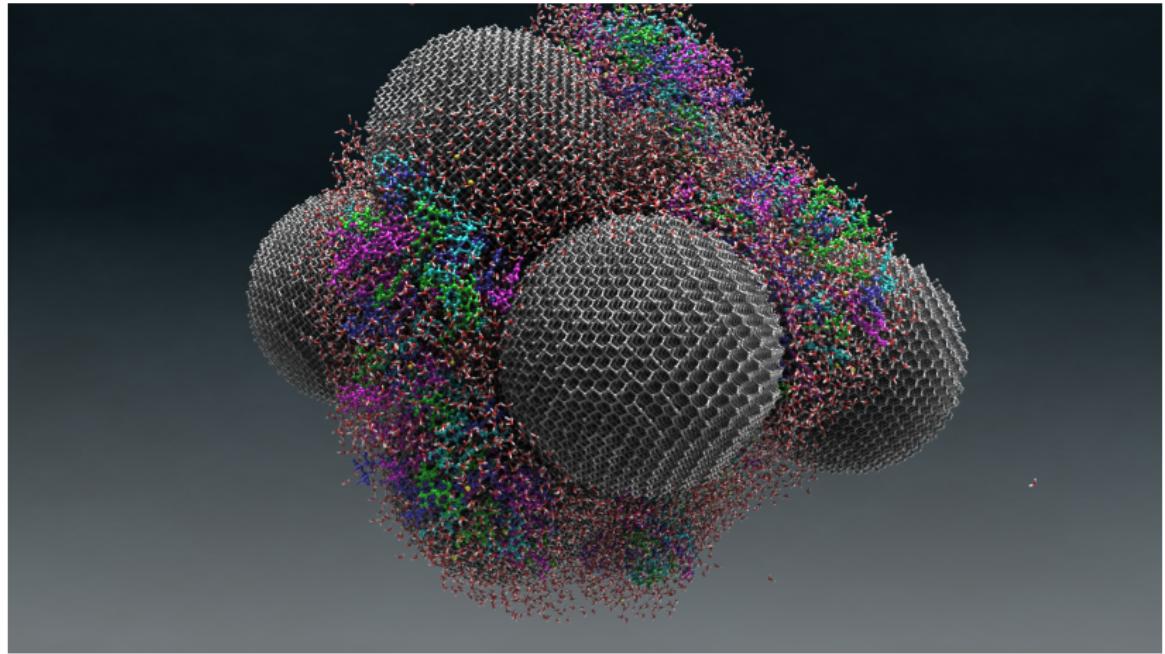
Diamonds That Deliver

- ▶ HPC simulations are used to solve complex problems such as drug delivery.
- ▶ Theory suggests that nanodiamonds are good delivery candidates.
- ▶ International team of ORNL researchers were able to simulate tRNA transfer without having to test on humans.
- ▶ This work was done on Titan.
- ▶



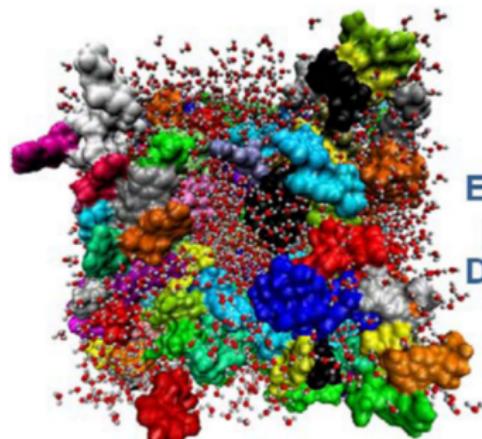
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Diamonds That Deliver



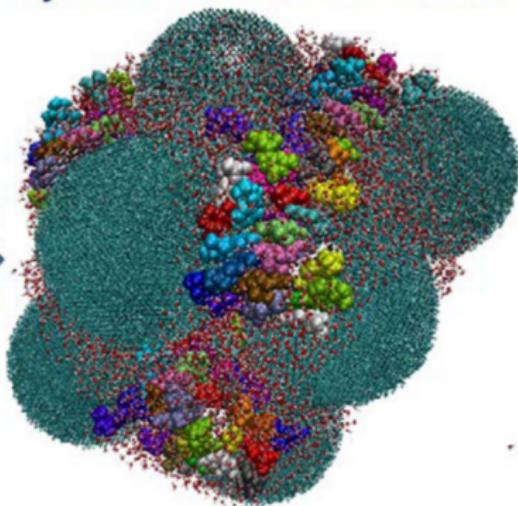
Diamonds That Deliver

Freestanding hydrated tRNA

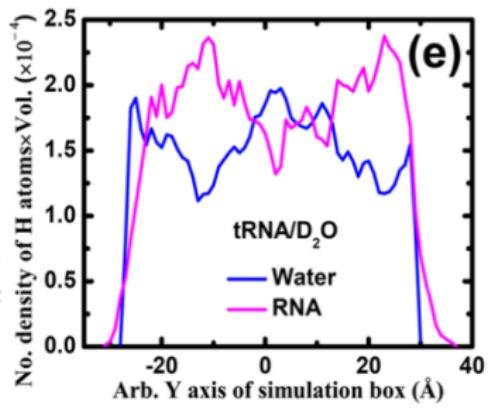
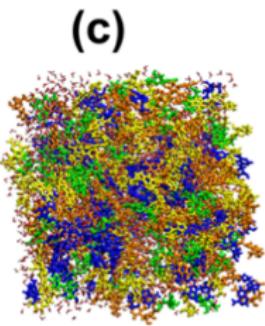
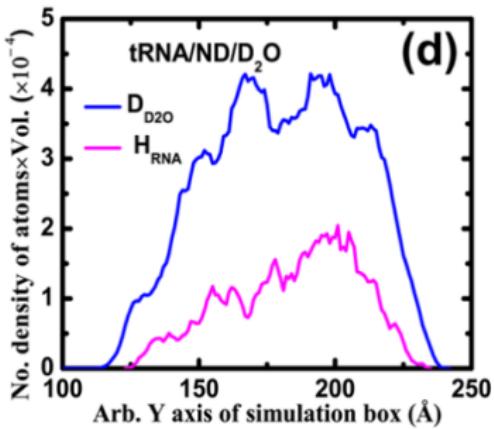
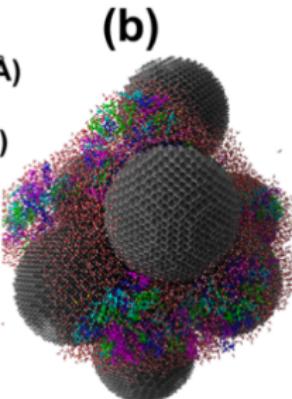
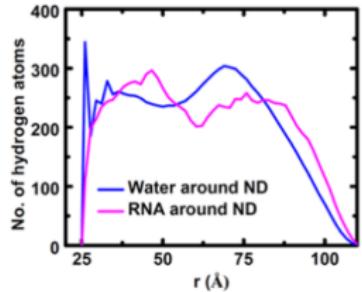
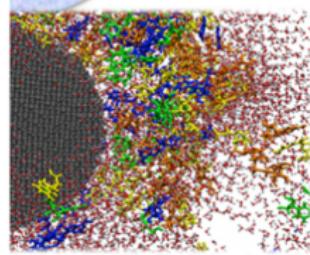
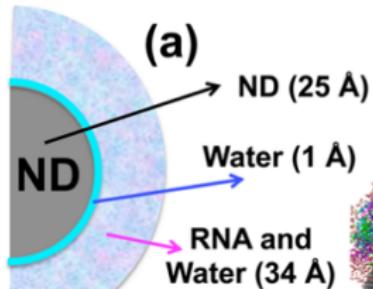


Enhanced
Dynamics

Hydrated tRNA on ND surfaces



Diamonds That Deliver



Diamonds That Deliver

- ▶ <https://www.youtube.com/watch?v=59428CbAXWE>
- ▶ <https://www.youtube.com/watch?v=w4wQGXfEoMg>

Diamonds That Deliver

- ▶ The visualizations are what lead to better understanding.
- ▶ Let's scientists "quickly" determine drug candidates and delivery mechanisms.
- ▶ These simulations helped inform scientists of the motions of tRNA and this helps them treat conditions such as cancer and genetic disorders.
- ▶ ORNL is currently using Summit to screen drugs for the Corona Virus.

Questions?